Domain decomposition for physics-informed neural networks and operators

Alexander Heinlein[1]

SIAM Conference on Computational Science and Engineering (CSE25), Fort Worth, Texas, U.S., March 3-7, 2025

[1]Delft University of Technology

Outline

1. FBPINNs – Multilevel domain decomposition-based architectures for physics-informed neural networks

   Based on joint work with

Victorita Dolean	(Eindhoven University of Technology)
Ben Moseley	(Imperial College London)
Siddhartha Mishra	(ETH Zürich)

2. Multilevel domain decomposition-based physics-informed deep operator networks

   Based on joint work with

Amanda A. Howard and **Panos Stinis**	(Pacific Northwest National Laboratory)

FBPINNs – Multilevel domain decomposition-based architectures for physics-informed neural networks

Physics-Informed Neural Networks (PINNs)

In the **physics-informed neural network (PINN)** approach introduced by **Raissi et al. (2019)**, a **neural network** is employed to **discretize a partial differential equation**

$$\mathcal{N}[u] = f, \quad \text{in } \Omega.$$

PINNs use a **hybrid loss function**:

$$\mathcal{L}(\boldsymbol{\theta}) = \omega_{\text{data}} \mathcal{L}_{\text{data}}(\boldsymbol{\theta}) + \omega_{\text{PDE}} \mathcal{L}_{\text{PDE}}(\boldsymbol{\theta}),$$

where ω_{data} and ω_{PDE} are **weights** and

$$\mathcal{L}_{\text{data}}(\boldsymbol{\theta}) = \frac{1}{N_{\text{data}}} \sum_{i=1}^{N_{\text{data}}} \left(u(\hat{\mathbf{x}}_i, \boldsymbol{\theta}) - u_i \right)^2,$$

$$\mathcal{L}_{\text{PDE}}(\boldsymbol{\theta}) = \frac{1}{N_{\text{PDE}}} \sum_{i=1}^{N_{\text{PDE}}} \left(\mathcal{N}[u](\mathbf{x}_i, \boldsymbol{\theta}) - f(\mathbf{x}_i) \right)^2.$$

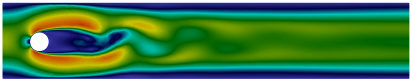
See also **Dissanayake and Phan-Thien (1994); Lagaris et al. (1998)**.

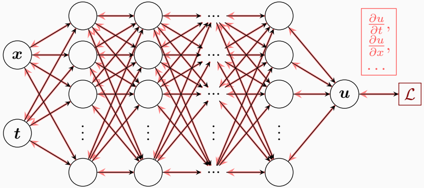
Advantages

- **"Meshfree"**
- **Small data**
- **Generalization properties**
- **High-dimensional problems**
- **Inverse** and **parameterized problems**

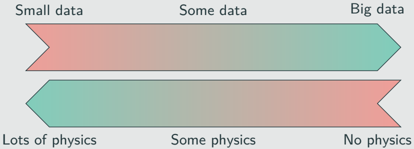
Drawbacks

- **Training cost** and **robustness**
- **Convergence not well-understood**
- **Difficulties with scalability** and **multi-scale problems**





Hybrid loss



- **Known solution values** can be included in $\mathcal{L}_{\text{data}}$
- **Initial and boundary conditions** are also included in $\mathcal{L}_{\text{data}}$

Scaling of PINNs for a Simple ODE Problem

Solve

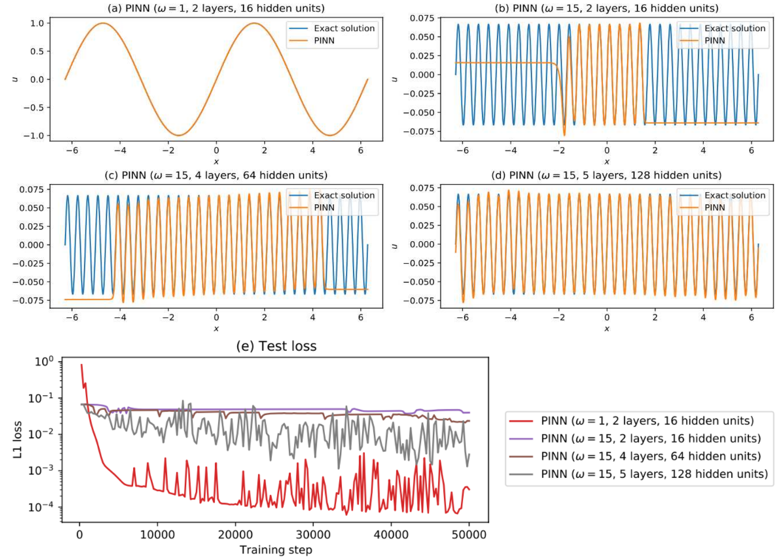
$$
\begin{aligned}
u' &= \cos(\omega \boldsymbol{x}), \\
u(0) &= 0,
\end{aligned}
$$

for different values of ω using **PINNs with varying network capacities**.

Scaling issues

- Large computational domains
- Small frequencies

Cf. **Moseley, Markham, and Nissen-Meyer (2023)**



(a) 321 free parameters

(d) 66 433 free parameters

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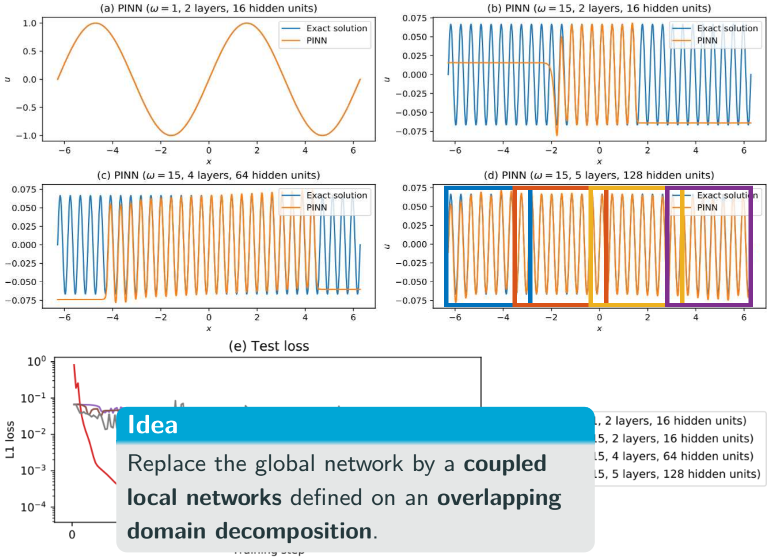


Idea

Replace the global network by a **coupled local networks** defined on an **overlapping domain decomposition**.

(a) 321 free parameters (d) 66 433 free parameters

Domain Decomposition Methods and Machine Learning – Literature

A **non-exhaustive literature overview**:

- **Machine Learning for adaptive BDDC, FETI–DP, and AGDSW**: Heinlein, Klawonn, Lanser, Weber (2019, 2020, 2021, 2021, 2021, 2022); Klawonn, Lanser, Weber (2024)
- **cPINNs, XPINNs**: Jagtap, Kharazmi, Karniadakis (2020); Jagtap, Karniadakis (2020)
- **Classical Schwarz iteration for PINNs or DeepRitz (D3M, DeepDDM, etc)**:: Li, Tang, Wu, and Liao (2019); Li, Xiang, Xu (2020); Mercier, Gratton, Boudier (arXiv 2021); Dolean, Heinlein, Mercier, Gratton (subm. 2024 / arXiv:2408.12198); Li, Wang, Cui, Xiang, Xu (2023); Sun, Xu, Yi (arXiv 2023, 2024); Kim, Yang (2023, 2024, 2024)
- **FBPINNs**, **FBKANs**: Moseley, Markham, and Nissen-Meyer (2023); Dolean, Heinlein, Mishra, Moseley (2024, 2024); Heinlein, Howard, Beecroft, Stinis (acc. 2024 / arXiv:2401.07888); Howard, Jacob, Murphy, Heinlein, Stinis (arXiv:2406.19662)
- **DDMs for CNNs**: Gu, Zhang, Liu, Cai (2022); Lee, Park, Lee (2022); Klawonn, Lanser, Weber (2024); Verburg, Heinlein, Cyr (subm. 2024)

An overview of the state-of-the-art in early 2021:

A. Heinlein, A. Klawonn, M. Lanser, J. Weber

Combining machine learning and domain decomposition methods for the solution of partial differential equations — A review

GAMM-Mitteilungen. 2021.

An overview of the state-of-the-art in mid 2024:

A. Klawonn, M. Lanser, J. Weber

Machine learning and domain decomposition methods – a survey

Computational Science and Engineering. 2024

Finite Basis Physics-Informed Neural Networks (FBPINNs)

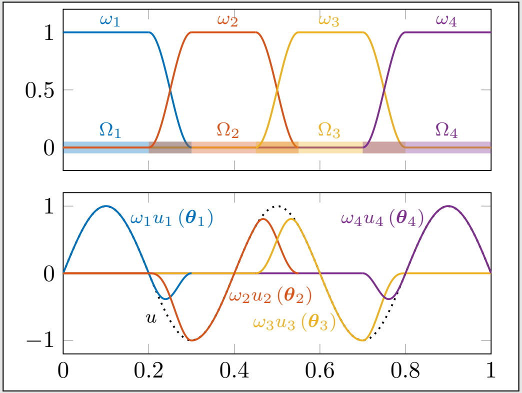
FBPINNs (Moseley, Markham, Nissen-Meyer (2023))

FBPINNs employ the **network architecture**

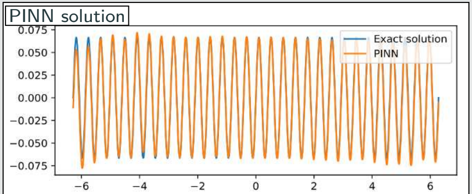
$$u(\theta_1, \ldots, \theta_J) = \sum\nolimits_{j=1}^{J} \omega_j u_j(\theta_j)$$

and the **loss function**

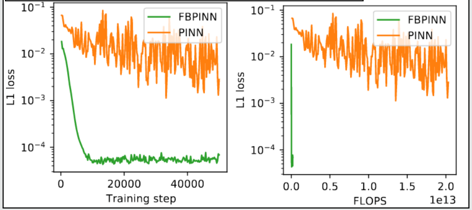
$$\mathcal{L} = \frac{1}{N} \sum\nolimits_{i=1}^{N} \left(n[\sum\nolimits_{x_i \in \Omega_j} \omega_j u_j](x_i, \theta_j) - f(x_i) \right)^2.$$



1D single-frequency problem



Moseley, Markham, Nissen-Meyer (2023)



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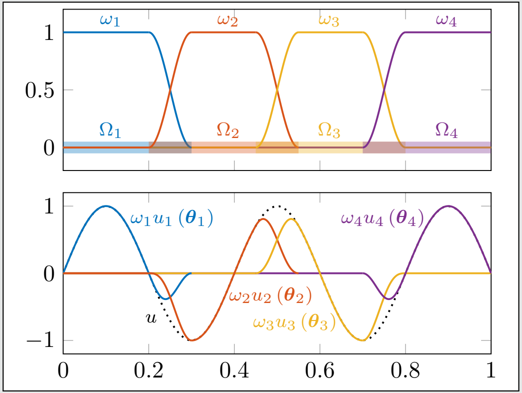

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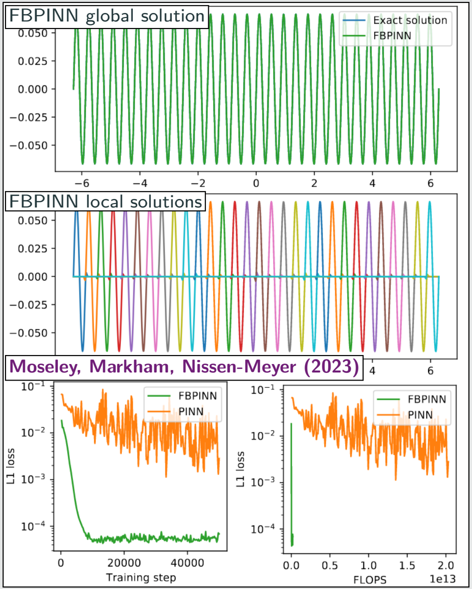
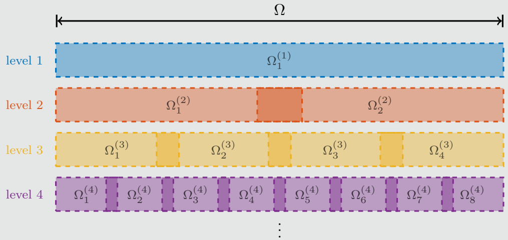


Multi-level FBPINNs (ML-FBPINNs)

ML-FBPINNs (**Dolean, Heinlein, Mishra, Moseley (2024)**) are based on a **hierarchy of domain decompositions:**



This yields the **network architecture**

$$u\left(\boldsymbol{\theta}_1^{(1)}, \ldots, \boldsymbol{\theta}_{J^{(L)}}^{(L)}\right) = \sum\nolimits_{l=1}^{L} \sum\nolimits_{i=1}^{N^{(l)}} \omega_j^{(l)} u_j^{(l)}\left(\boldsymbol{\theta}_j^{(l)}\right)$$

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Multi-Frequency Problem

Let us now consider the **two-dimensional multi-frequency Laplace boundary value problem**

$$\begin{aligned} -\Delta u &= 2 \sum_{i=1}^{n} (\omega_i \pi)^2 \sin(\omega_i \pi x) \sin(\omega_i \pi y) && \text{in } \Omega, \\ u &= 0 && \text{on } \partial\Omega, \end{aligned}$$

with $\omega_i = 2^i$.

For increasing values of n, we obtain the **analytical solutions**:

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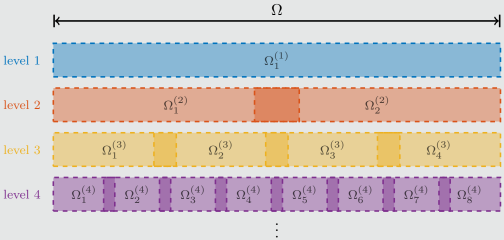

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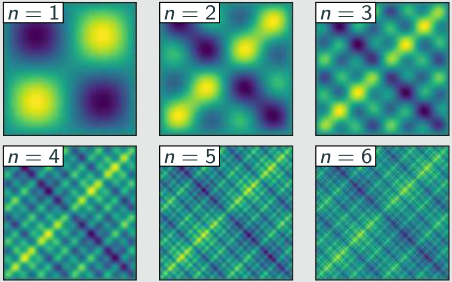
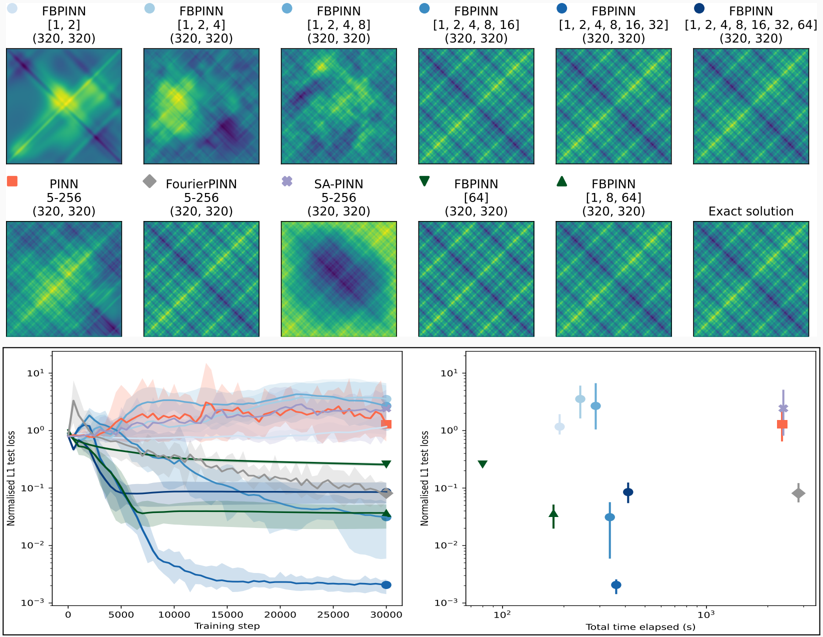
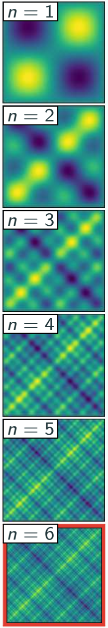
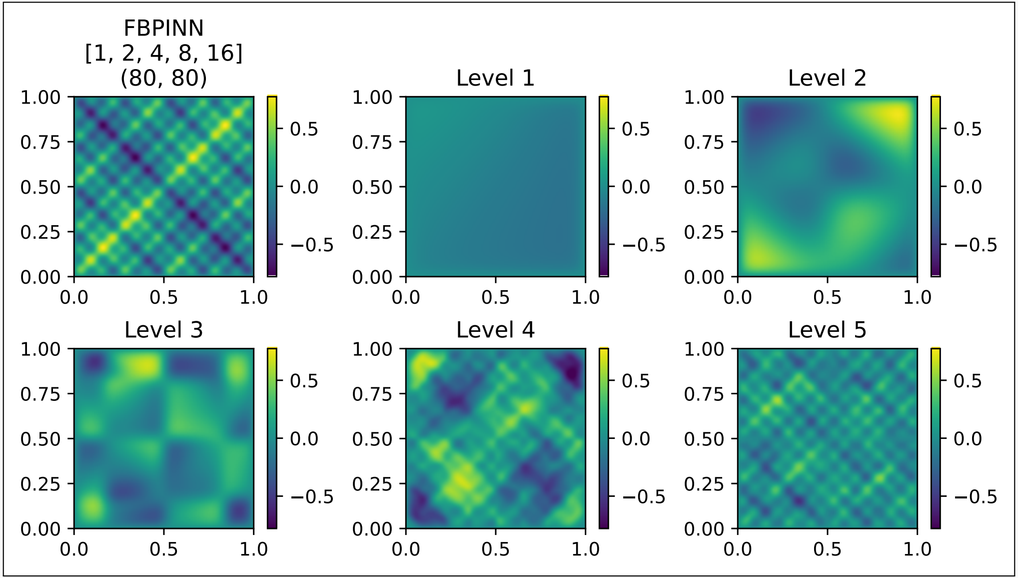


Multi-Level FBPINNs for a Multi-Frequency Problem – Strong Scaling



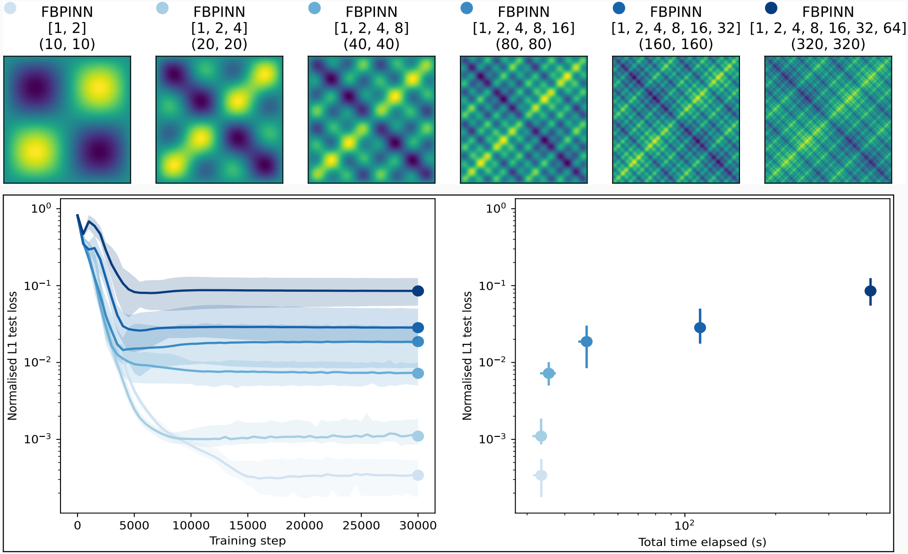


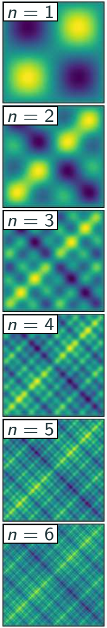
Multi-Frequency Problem – What the FBPINN Learns



Cf. **Dolean, Heinlein, Mishra, Moseley (2024)**.

Multi-Level FBPINNs for a Multi-Frequency Problem – Weak Scaling



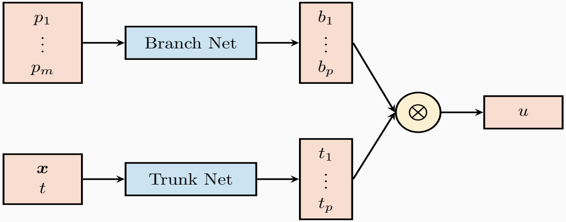


→ Details and results for the Helmholtz equation can be found in **Dolean, Heinlein, Mishra, Moseley (2024)**.

Multilevel domain decomposition-based physics-informed deep operator networks

Deep Operator Networks (DeepONets / DONs)

Neural operators learn operators between function spaces using neural networks. Here, we learn the **solution operator** of a initial-boundary value problem parametrized with $p_1, \ldots, p_m$ using **DeepONets** as introduced in **Lu et al. (2021)**.



Single-layer case

The DeepONet architecture is based on the **single-layer case** analyzed in **Chen and Chen (1995)**. In particular, the authors show **universal approximation properties for continuous operators**.

The architecture is based on the following ansatz for presenting the parametrized solution

$$u_{(p_1,\ldots,p_m)}(\boldsymbol{x}, t) = \sum\nolimits_{i=1}^{p} \underbrace{b_i(p_1, \ldots, p_m)}_{\text{branch}} \cdot \underbrace{t_i(\boldsymbol{x}, t)}_{\text{trunk}}$$

Physics-informed DeepONets

DeepONets are **compatible with the PINN approach** but **physics-informed DeepONets (PI-DeepONets)** are challenging to train.

Other operator learning approaches

- **FNOs**: **Li et al. (2021)**
- **PCA-Net**: **Bhattacharya et al. (2021)**
- **Random features**: **Nelsen and Stuart (2021)**
- **CNOs**: **Raonić et al. (arXiv 2023)**

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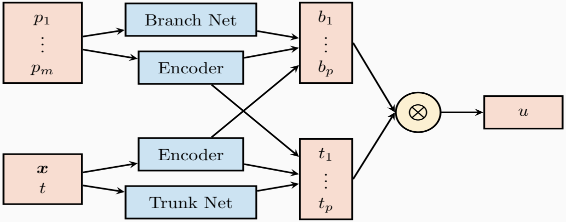

Modified architecture

In our numerical experiments, we employ the **modified DeepONet architecture** introduced in **Wang, Wang, and Perdikaris (2022)**.

The architecture is based on the following ansatz for presenting the parametrized solution

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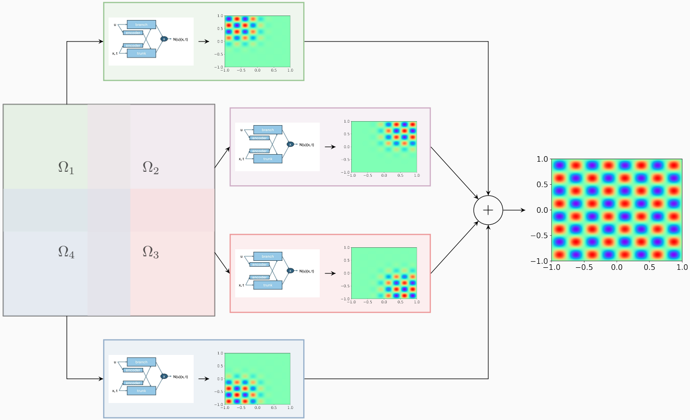


Howard, Heinlein, Stinis (in prep.)

Variants:

Shared-trunk FBDONs (ST-FBDONs)

The trunk net learns spatio-temporal basis functions. In ST-FBDONs, we use the **same trunk network for all subdomains**.

Stacking FBDONs

Combination of the **stacking multifidelity approach** with FBDONs.

Heinlein, Howard, Beecroft, Stinis (acc. 2024/arXiv:2401.07888)

FBDONs – Pendulum

Pendulum problem

$$\frac{ds_1}{dt} = s_2, \qquad t \in [0, T],$$
$$\frac{ds_2}{dt} = -\frac{b}{m}s_2 - \frac{g}{L}\sin(s_1), \qquad t \in [0, T],$$

where $m = L = 1$, $b = 0.05$, $g = 9.81$, and $T = 20$.

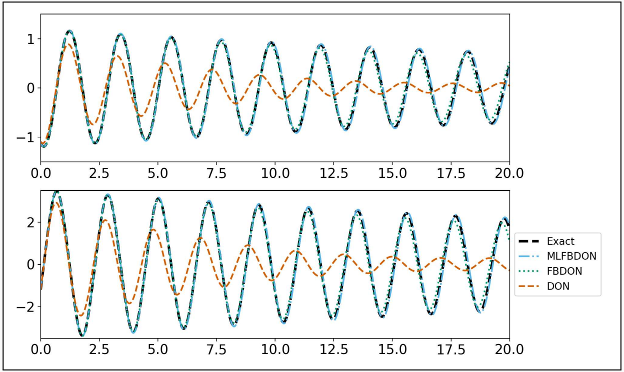
Parametrization

Initial conditions:

$$s_1(0) \in [-2, 2] \qquad s_2(0) \in [-1.2, 1.2]$$

$s_1(0)$ and $s_2(0)$ are the also inputs of the branch network.

Training on 50 k different configurations



Mean rel. l_2 error on 100 config.	
DeepONet	0.94
FBDON (32 subd.)	0.84
MLFBDON ([1, 4, 8, 16, 32] subd.)	0.27

Cf. **Howard, Heinlein, Stinis (in prep.)**

FBDONs – Wave Equation

Wave equation

$$\frac{d^2 s}{dt^2} = 2\frac{d^2 s}{dx^2}, \qquad (x,t) \in [0,1]^2$$

$$s_t(x,0) = 0, x \in [0,1], \quad s(0,t) = s(1,t) = 0,$$

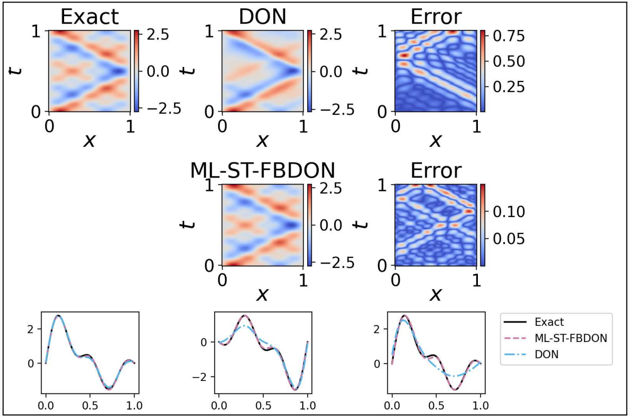
Solution: $s(x,t) = \sum_{n=1}^{5} b_n \sin(n\pi x)\cos(n\pi\sqrt{2}t)$

Parametrization

Initial conditions for s parametrized by $b = (b_1, \ldots, b_5)$ (normally distributed):

$$s(x,0) = \sum_{n=1}^{5} b_n \sin(n\pi x) \quad x \in [0,1]$$

Training on 1 000 random configurations.

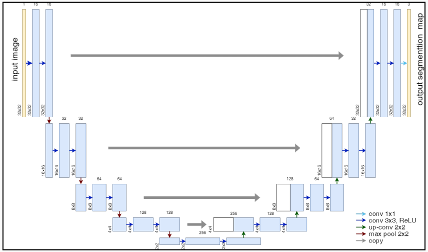


Mean rel. l_2 error on 100 config.	
DeepONet	0.30 ± 0.11
ML-ST-FBDON ([1, 4, 8, 16] subd.)	0.05 ± 0.03
ML-FBDON ([1, 4, 8, 16] subd.)	0.08 ± 0.04

→ Sharing the trunk network does not only save in the number of parameters but even yields **better performance**

Cf. **Howard, Heinlein, Stinis (in prep.)**

Domain Decomposition-Based U-Net Architecture

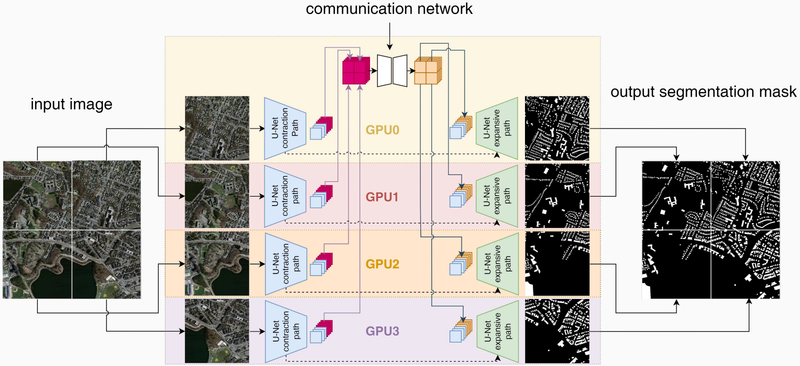


name	mem. feature maps		mem. weights	
	# of values	MB	# of values	MB
input block	268 M	1 024.0	38 848	0.148
encoder blocks	314 M	1 320	18 M	72
decoder blocks	754 M	3880	12 M	47
output block	3.1 M	12.0	195	0.001

Most memory in the U-Net is used by feature maps, **not weights**

→ **Decompose feature maps** to **distribute memory consumption**.

Cf. **Verburg, Heinlein, Cyr (subm. 2024).**



CWI Research Semester: Synergies in Numerical Linear Algebra and Machine Learning

Co-organizers: Victorita Dolean (TU/e), Alexander Heinlein (TU Delft), Benjamin Sanderse (CWI), Jemima Tabbeart (TU/e), Tristan van Leeuwen (CWI)

- **Autumn School** (October 27–31, 2025):
  - Chris Budd (University of Bath)
  - Ben Moseley (Imperial College London)
  - Gabriele Steidl (Technische Universität Berlin)
  - Andrew Stuart (California Institute of Technology)
  - Andrea Walther (Humboldt-Universität zu Berlin)
- **Workshop** (December 1–3, 2025):
  - 3 days with plenary talks (academia & industry) and an industry panel
  - Confirmed plenary speakers:
    - Marta d'Elia (Meta)
    - Benjamin Peherstorfer (New York University)
    - Andreas Roskopf (Fraunhofer Institute)

Centrum Wiskunde & Informatica

Join us for inspiring talks, hands-on sessions, and industry collaboration!

Multilevel Finite Basis Physics Informed Neural Networks (ML-FBPINNs)

- **Schwarz domain decomposition architectures** improve the scalability of PINNs to **large domains** / **high frequencies**, keeping the complexity of the local networks low.
- As classical domain decomposition methods, **one-level FBPINNs** are not scalable to large numbers of subdomains; **multilevel FBPINNs** enable scalability.

Extension to Deep Operator Networks (DeepONets)

- **DeepONets** offer efficient predictions for **parametrized problems** but can struggle with training a good global basis (trunk net), especially for **multiscale problems**.
- **Domain decomposition-based architectures** can significantly enhance performance by **localizing the learning process**.

Thank you for your attention!

Topical Activity Group

Scientific Machine Learning